Title	Introduction to Quantum Molecular Modelling
Credits	2.5
Semester	2 (Year 1)
Level	4
Coordinator	Prof. Graeme Watson

Indicative Module Descriptor:

The module aims to give students an overview of the principles underlying the standard quantum mechanics techniques for simulation the structure and properties of molecular systems. This will include basic theory behind the approaches as well as practical aspect such as basis set choice. This course will include the performance of different approaches such HF, DFT, MP2, CI, CC.

Indicative Learning Outcomes

On successful completion of this module, students should:

- Understanding of potential energy surfaces, important points, basic optimisation and molecular dynamics.
- Understand at a basic level the Hartree-Fock approach its approximations
- Know the definition of correlation, where it is important and the key aspects of post-HF approaches which include correlation (MP2, CI, MCSCF, CC)
- Basic understanding of Density Functional Theory and its differences compared to wavefunction approaches (i.e. Hartree-Fock)
- Detailed knowledge of different types and naming of basis sets including minimal, double /triple zeta, split-valence, polarisation and diffuse functions.
- Be able to choose an appropriate methods for a particular problem based on analysis of the performance of different approaches fro different problems.
- Prepare a Gaussian03 input file, include basis set, and analyse the results (using Gaussian03 for windows)

Workload:	50		
Class Contact: Lectures	12		
Laboratory	3		
Specified Assignments	15		
Laboratory write up	10		
Background reading	10		
Assessment	type	%	timing
Examination	Written exam (2hr)	35	End Yr 1
Assignments		35	Continuous
Laboratory		30	

Students are required to:

1. Answer 5 assignment sheets (one at the end of every 2 hours of lectures) (10) (35%)
2. Complete a laboratory and prepare a written report (4+6 = 10) (30%)
3. Pass (35%) a written examination. (2hr)

Students will either pass or fail the module on basis of satisfactory or unsatisfactory completion of the assigned tasks.